ELSEVIER

J. Non-Newtonian Fluid Mech. 149 (2008) 40–55

Journal of Non-Newtonian Fluid Mechanics

www.elsevier.com/locate/jnnfm

Consistent closure schemes for statistical models of anisotropic fluids

Martin Kröger [a,*], Amine Ammar [b], Francisco Chinesta [c]

[a] *Polymer Physics, ETH Zurich, Department of Materials, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland*
[b] *Laboratoire de Rhéologie, UMR 5520 CNRS-UJF-INPG, 1301 Rue de la Piscine, BP 53 Domaine Universitaire, F-38041 Grenoble Cedex 9, France*
[c] *LMSP UMR 8106 CNRS-ENSAM-ESEM, 151 Boulevard de l'Hôpital, F-75013 Paris, France*

Received 30 October 2006; received in revised form 7 April 2007; accepted 19 May 2007

Abstract

We propose a rational approach to approximating the various alignment tensors. It preserves the correct symmetry and leads to consistent results. For the case of uniaxial nematic fluids, the decoupling approximation for a tensor of rank n involves $(n-2)/2$ scalar functions $S_n(S_2)$ in terms of a scalar argument S_2, with $S_n(0)=0$ and $S_n(1)=1$. Nothing else can be concluded about the mathematical relationship between moments of the distribution function, and in particular, all consistent decoupling approximations for fourth-order moment in terms of second-order moments can be characterized by a single $S_4(S_2)$ function. We propose using the simple model dependent convex shaped equilibrium relationship between S_4 and S_2 to characterize new (and simple) decoupling approximations K-I and K-II for the biaxial (including uniaxial) phase. In order to test the new against earlier proposed approximations rigorously, and to discuss consistency issues, we solve the Hess–Doi Fokker–Planck equation for nematic and nematic-discotic liquid crystals efficiently for a wide range of (2300 distinct) possible conditions including mixed shear and elongational flows, diverse field strengths, and molecular shapes. As a result, we confirm the closures K-I and K-II with correct tensorial symmetry; they are valid under arbitrary conditions to high precision, exact in the isotropic and totally aligned phases, improve upon earlier parameter-free closures in particular in the temperature regime $T \in [0.6, \infty] \times T_{\mathrm{NI}}$ with the nematic-isotropic transition temperature T_{NI} (or alternatively, for mean-field strengths $U \in [0, 8]$). K-II performs as good as the so-called Bingham closure, which usually requires 30 empirical coefficients, while K-I and K-II are essentially parameter-free, and their quality can be expected to be insensitive to the particular model.
© 2007 Elsevier B.V. All rights reserved.

PACS: 61.30.Gd; 61.30.Cz; 47.50.+d

Keywords: Anisotropic fluids; Closure schemes; Nematic fluids; Alignment tensors; Ferrofluids; Numerical solution of Fokker–Planck equation

1. Introduction

Anisotropic fluids consist of particles or molecules that can be aligned by flow and external fields. One approach to modeling such fluids is to introduce a set of unit vectors fields, usually called directors, that represent the preferred directions of the particle orientations. If there are fluctuations in the particle orientations, however, the alignment of the particles is not perfect. In this case, the directors represent the particle orientations in an averaged, macroscopic sense. This director approach has been quite successful in modeling low molecular weight liquid crystals where the degree of alignment is generally constant [1–4], and in modelling ferrofluids [5–8].

For some anisotropic fluids, such as liquid crystal polymers, particle fluctuations play an important role in the overall properties. An alternative description that explicitly takes into account fluctuations in particle orientations and the resulting variable degree of alignment is a statistical one with a distribution function providing the information for the particle orientations. The orientation distribution function satisfies an evolution equation (for a review see, e.g., [9]). In general, however, this evolution equation can be solved only numerically. And for most microstructural models, such as the Hess–Doi model for rigid, rod-like liquid crystal polymers [10,11], the complete numerical solution of the orientation distribution function at present is quite prohibitive and impractical [12] for common applications, cf. [13] for solution methods. Approximative solutions are also available [14–16] which allow to characterize the spatiotemporal behavior of liquid crystals [17,18].

Alternatively to solving directly for the distribution function, one can reformulate the statistical model in terms of a

* Corresponding author.
E-mail address: mk@mat.ethz.ch (M. Kröger).

0377-0257/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnnfm.2007.05.007

hierarchy of higher tensorial moments of the alignment (the so-called alignment tensors) and then solve the resulting evolution equations for the alignment tensors. The alignment tensors are useful since their principal directions are related to the macroscopic directors and their principal values are related to the scalar order parameters that characterize the variable degree of alignment. Since there is in general an *infinite hierarchy* of coupled evolution equations for the alignment tensors, this problem is also computationally difficult, so that various closure schemes have been introduced to relate higher moments of the alignment to lower moments. The most common closure schemes relate the fourth-order alignment tensor to the second-order one. Such approximations simplify considerably the effort to obtain the macroscopic alignment, and a large amount of work has been invested in studying them. The proposed schemes include linear [19] and quadratic closure [10,20], interpolation between the limiting cases of weak alignment and perfect alignment [21], truncation of the evolution equations after a certain order [9,10,14–16,22,23], maximum entropy method [24], time-structure invariance criteria [25,26], and specification of an a priori form of the orientation distribution function [27–31].

These closure schemes have been proposed often on an ad hoc basis and are sometimes inconsistent with the exact equations based on the orientation distribution function [12,32,33]. For example, in the Doi and Edwards [20] model the quadratic closure gives an incorrect expression for the fourth-order alignment tensor in the isotropic phase as well as an incorrect orientation of the director in the uniaxial phase, while being still compatible with time-structure invariance criteria [25]. Some closure schemes also commonly lead to pathological results for certain parameter ranges [12,34]. One reason for this inconsistency is that the various schemes yield an overdetermined system of equations for the principal directions and principal values of the alignment tensors. In particular, any scheme that approximates both principal values and principal directions can lead to an overdetermined system.

The purpose of this paper is to show how this overdeterminacy arises and, most importantly, how to formulate consistent closure schemes so that it does not arise. This leads us to propose new and simple closure schemes independent of the particular microstructural model. Our procedure is based on the representation of the alignment tensors in terms of their principal values and principal directions. These representations show that only the independent *principal values* of the alignment tensors need to be approximated in a closure scheme. For example, specifying the principal values of the fourth-order alignment tensor in terms of the principal values of the second-order alignment tensor leads to a consistent second-order closure scheme. By avoiding any assumptions on the principal directions, our procedure maintains the correct symmetry and preferred orientations, thus leading to consistent, non-pathological results. Although our procedure is quite general, for simplicity we treat in detail only the second to fourth-order alignment tensors.

We begin with a review of measures of alignment for anisotropic fluids. The symmetry is conveniently divided into three cases according to the number of distinct principal values: isotropic, uniaxial and biaxial. We examine all three cases and discuss consistent closure schemes for each case. In particular, for the uniaxial case, a consistent closure scheme requires specifying only a single scalar parameter. For the biaxial case, three scalar parameters must be specified. Furthermore, the choice of these three relations is strongly restricted by the requirement that the fourth-order alignment tensor be expressible in terms of the second-order alignment tensor. We also show that a modified quadratic closure relation can hold for all three types of symmetry, which is important for materials that can exhibit all three types of symmetry, such as liquid crystal polymers in complex flows. Our results demonstrate, however, that most commonly used closure schemes are inconsistent and, hence, lead to incorrect results. An exception, although, is the scheme that postulates an a priori form for the orientation distribution function.

As an illustration of our procedure, we apply it to the Hess–Doi model for rigid, rod-like polymers and to ferrofluids. The results can be useful for simulating complex flows such as those arising in the injection molding of liquid crystalline polymers into high strength parts.

2. Orientational distribution function

For uniaxial-shaped particles with symmetry axis $\boldsymbol{u}$, the orientational (part of a eventually space and time-dependent) distribution function $f(\boldsymbol{u})$ with $u^2 = 1$ can be expanded in terms of Cartesian symmetric traceless (anisotropic, irreducible) tensors $\boldsymbol{u}_{[n]} \equiv \overline{\boldsymbol{u}_{(l)}}$ of rank n, with $\boldsymbol{u}_{(n)} \equiv \boldsymbol{u}\boldsymbol{u}\ldots\boldsymbol{u}$ the n-fold tensorial product of vector $\boldsymbol{u}$, the symbol $\overline{\ldots}$ denoting the anisotropic part, and the tensorial coefficients in front of the $\boldsymbol{u}_{[n]}$'s are determined by multiplying f with $\boldsymbol{u}_{[n]}$ and subsequent integration over the unit sphere, to yield

$$f(\boldsymbol{u}) = \frac{1}{4\pi}\left(1 + \sum_{n=1}^{\infty}\langle\zeta_n \boldsymbol{u}_{[n]}\rangle \odot^n (\zeta_n \boldsymbol{u}_{[n]})\right) = \frac{1}{4\pi}\sum_{n=0}^{\infty}\zeta_n^2 \boldsymbol{a}_{(n)}\odot^n \boldsymbol{u}_{[n]}, \tag{1}$$

where $\odot^l$ denotes an n-fold contraction and $\boldsymbol{a}_{[l]} \equiv \langle \boldsymbol{u}_{[l]}\rangle$ the n th rank alignment tensor. The constant $(4\pi)^{-1}$ ensures proper normalization $\langle 1\rangle = 1$, and the average $\langle\ldots\rangle$ is defined through $\langle\ldots\rangle \equiv \int \ldots f(\boldsymbol{u})\,\mathrm{d}^2u$. The prefactor

$$\zeta_n = \sqrt{\frac{(2n+1)!!}{n!}}, \tag{2}$$

with $k!! = k(k-2)(k-4)\ldots$ is immediately derived using the identity [9]

$$\frac{1}{4\pi}\int \boldsymbol{u}_{[k]}\boldsymbol{u}_{[n]}\,\mathrm{d}^2u = \frac{n!}{(2n+1)!!}\delta_{kn}\boldsymbol{\Delta}^{(n)}, \tag{3}$$

where $\boldsymbol{\Delta}^{(n)}$ is the isotropic tensor [9,35]– and projector – of rank n with the feature $\boldsymbol{\Delta}^{(n)}\odot^n \boldsymbol{a}_{(n)} = \boldsymbol{a}_{[n]}$ and just $\boldsymbol{\Delta}^{(0)} = 1$ is needed here to prove (2). Within the statistical approach to the dynamics of anisotropic fluids, the distribution function obeys a Fokker–Planck (FP) equation from which coupled equations of moments (including anisotropic moments—the alignment

Download English Version:

https://daneshyari.com/en/article/671524

Download Persian Version:

https://daneshyari.com/article/671524

Daneshyari.com